



chain nodes :

1 2 3 4 5 7

ring nodes :

9 10 11 12 13 14 16 17 18 19 20 21 22 23 24 25 26 27 30 31 32 33 34 35  
 36 37 38 40 41 42 43 44 45 46 47 48 50 51 52 53 54 55 56 57 58 60 61 62  
 63 64 65 66 67 68 71 72 73 74 75 76 77 78 79 82 83 84 85 86 87 88 89 90  
 92 93 94 95 96 97 98 99 100 102 103 104 105 106 107 108 109 110 112 113 114  
 115 116 117 119 120 121 122 123 124 125 126 127 128 129 130 132 133 134 135  
 136 137 138 139 140

chain bonds :

1-2 2-3 2-4 4-5

ring bonds :

9-10 9-14 10-11 11-12 11-16 12-13 12-18 13-14 16-17 17-18 19-20 19-24 20-21 21-22  
 21-25 22-23 22-27 23-24 25-26 26-27 30-31 30-35 31-32 32-33 32-36 33-34 33-38  
 34-35 36-37 37-38 40-41 40-45 41-42 42-43 42-46 43-44 43-48 44-45 46-47 47-48  
 50-51 50-55 51-52 52-53 52-56 53-54 53-58 54-55 56-57 57-58 60-61 60-65 61-62  
 62-63 62-66 63-64 63-68 64-65 66-67 67-68 71-72 71-76 72-73 73-74 73-77 74-75  
 74-79 75-76 77-78 78-79 82-83 82-87 83-84 84-85 84-88 85-86 85-90 86-87 88-89  
 89-90 92-93 92-97 93-94 94-95 94-98 95-96 95-100 96-97 98-99 99-100 102-103 102-107  
 103-104 104-105 104-108 105-106 105-110 106-107 108-109 109-110 112-113 112-117  
 113-114 114-115 114-119 115-116 115-121 116-117 119-120 120-121 122-123 122-127  
 123-124 124-125 124-128 125-126 125-130 126-127 128-129 129-130 132-133 132-137  
 133-134 134-135 134-138 135-136 135-140 136-137 138-139 139-140

exact/norm bonds :

1-2 2-3 2-4 4-5 11-16 12-18 16-17 17-18 21-25 22-27 25-26 26-27 32-36 33-38 36-37  
 37-38 42-46 43-48 46-47 47-48 52-56 53-58 56-57 57-58 62-66 63-68 66-67 67-68  
 73-77 74-79 77-78 78-79 84-88 85-90 88-89 89-90 94-98 95-100 98-99 99-100 104-108  
 105-110 108-109 109-110 114-119 115-121 119-120 120-121 124-128 125-130 128-129  
 129-130 134-138 135-140 138-139 139-140

normalized bonds :

9-10 9-14 10-11 11-12 12-13 13-14 19-20 19-24 20-21 21-22 22-23 23-24 30-31 30-35  
 31-32 32-33 33-34 34-35 40-41 40-45 41-42 42-43 43-44 44-45 50-51 50-55 51-52  
 52-53 53-54 54-55 60-61 60-65 61-62 62-63 63-64 64-65 71-72 71-76 72-73 73-74  
 74-75 75-76 82-83 82-87 83-84 84-85 85-86 86-87 92-93 92-97 93-94 94-95 95-96  
 96-97 102-103 102-107 103-104 104-105 105-106 106-107 112-113 112-117 113-114 114-115  
 115-116

116-117 122-123 122-127 123-124 124-125 125-126 126-127 132-133 132-137  
133-134 134-135 135-136 136-137  
isolated ring systems :  
containing 9 : 19 : 30 : 40 : 50 : 60 : 71 : 82 : 92 : 102 : 122 : 132 :

G2:[\*1],[\*2],[\*3],[\*4],[\*5],[\*6]

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 7:Atom 9:Atom 10:CLASS 11:Atom 12:Atom 13:Atom  
14:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 22:CLASS 23:Atom 24:Atom  
25:Atom 26:Atom 27:Atom 30:Atom 31:Atom 32:Atom 33:Atom 34:Atom 35:Atom 36:Atom  
37:Atom 38:Atom 40:Atom 41:Atom 42:Atom 43:Atom 44:Atom 45:Atom 46:Atom 47:Atom  
48:Atom 50:Atom 51:Atom 52:Atom 53:Atom 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom  
60:Atom 61:Atom 62:Atom 63:Atom 64:Atom 65:Atom 66:Atom 67:Atom 68:Atom 71:Atom  
72:CLASS 73:Atom 74:Atom 75:Atom 76:Atom 77:Atom 78:Atom 79:Atom 82:Atom 83:Atom  
84:Atom 85:Atom 86:Atom 87:Atom 88:Atom 89:Atom 90:Atom 92:Atom 93:Atom 94:Atom  
95:Atom 96:Atom 97:Atom 98:Atom 99:Atom 100:Atom 102:Atom 103:Atom 104:Atom 105:Atom  
106:Atom 107:Atom 108:Atom 109:Atom 110:Atom 112:Atom 113:Atom 114:Atom 115:Atom  
116:Atom 117:Atom 119:Atom 120:Atom 121:Atom 122:Atom 123:Atom 124:Atom 125:Atom  
126:Atom 127:Atom 128:Atom 129:Atom 130:Atom 132:Atom 133:Atom 134:Atom 135:Atom  
136:Atom 137:Atom 138:Atom 139:Atom 140:Atom

Generic attributes :

5:  
Saturation : Unsaturated  
Number of Carbon Atoms : less than 7  
Type of Ring System : Monocyclic  
7:  
Saturation : Unsaturated  
Number of Carbon Atoms : less than 7  
Number of Hetero Atoms : Exactly 1  
Type of Ring System : Monocyclic

Element Count :

Node 5: Limited  
C,C5-6  
N,N0-1

Node 7: Limited  
C,C5  
N,N1